Simulation Studies of Grain Boundary Diffusion in NiAl

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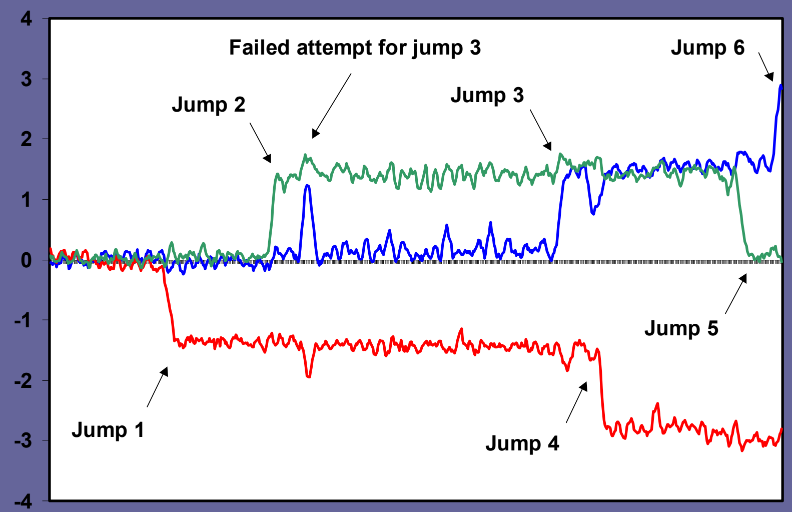
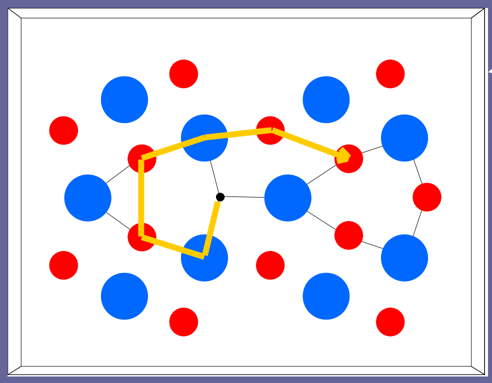
Direct molecular dynamics simulations of the diffusion process in ordered B2 NiAl at high temperature were performed using an embedded atom interatomic potential.
Diffusion occurs through a variety of cyclic mechanisms that accomplish the motion of the vacancy through nearest neighbor jumps restoring order to the alloy at the end of the cycle.
We studied the detailed time evolution of the jump sequence in these cyclic mechanisms. The traditionally postulated six-jump cycle is only one of the various cycles observed and some of these are quite complex.
We also identified the most favorable vacancy diffusion paths along a special coincident site grain boundary.
The project also involved the study of the atomistic structures of more general grain boundaries.

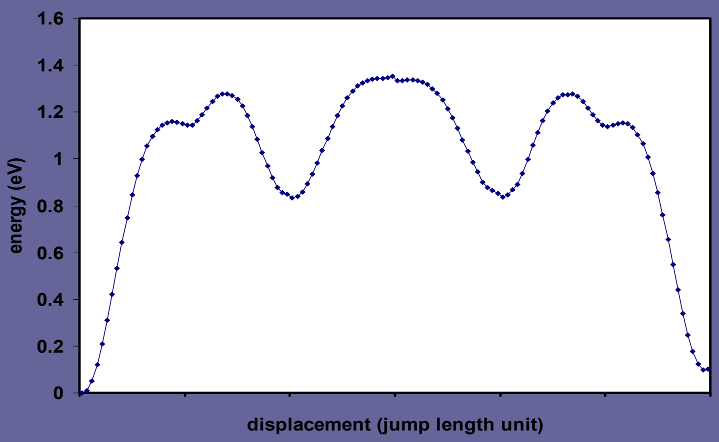


Detailed sequence of correlated jumps for a Ni vacancy cycle (above) and the corresponding energy barrier (below)



A favorable vacancy path for grain boundary diffusion

Al Ni path



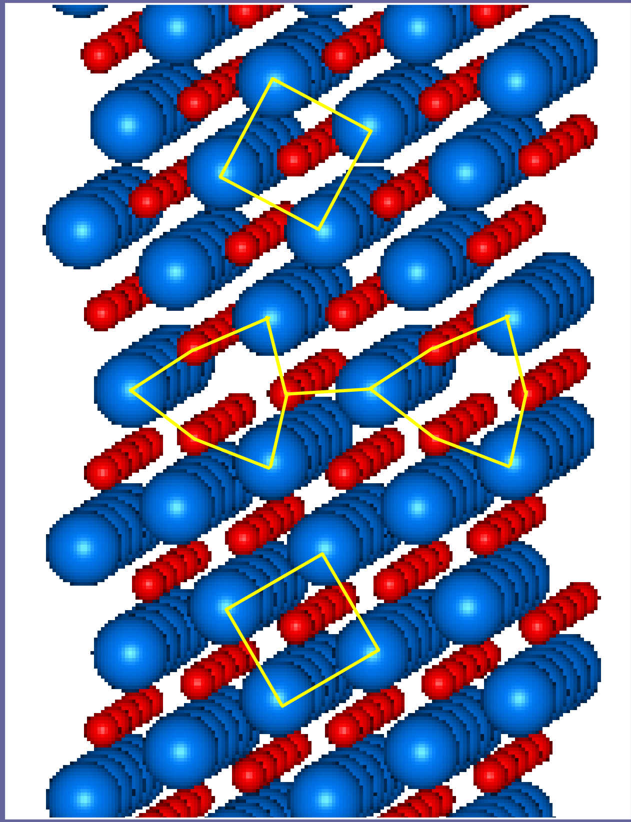
Educational:

The research results are incorporated into our curriculum in the teaching of basic diffusion mechanisms topics as well as grain boundary structure.

This was implemented in the framework developed as part of a combined research and curriculum (CRCD) development grant.

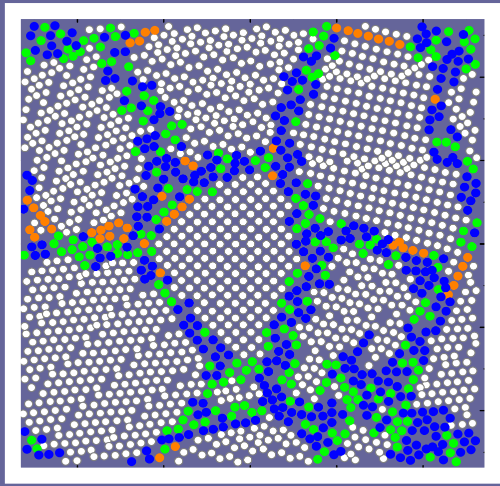
Collaborators:

Y. Mishin (George Mason)
D.A. Papaconstantopoulos (NRL)
H. van Swingenhoven (PSI, Switzerland)



Visualization of the structure of a special coincident site grain boundary .

Al Ni unit cells and structural units of the grain boundary



Digital polycrystalline sample used in studying the structure of random boundaries and in teaching topics related to the defect structure of metallic materials